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Avoiding the Bloat with Stochastic Grammar-based Genetic Programming

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Abstract. The application of Genetic Programming to the discovery of empirical laws is often impaired by the huge size of the search space, and consequently by the computer resources needed. In many cases, the extreme demand for memory and CPU is due to the massive growth of non-coding segments, the introns. The paper presents a new program evolution framework which combines distribution-based evolution in the PBIL spirit, with grammar-based genetic programming; the information is stored as a probability distribution on the grammar rules, rather than in a population. Experiments on a real-world like problem show that this approach gives a practical solution to the problem of intron growth.

1 Introduction

This paper is concerned with the use of Genetic Programming (GP) [1,2] for the automatic discovery of empirical laws. Although GP is widely used for symbolic regression [3,4], it suffers from two main limitations. One first limitation is that canonical GP offers no way to incorporate domain knowledge besides the set of operators, despite the fact that the knowledge-based issues of Evolutionary Computation are widely acknowledged [5,6].

In a previous work [7] was described a hybrid scheme combining GP and context free grammars (CFGs). First investigated by Gruau [8] and Whigham [9], CFG-based GP allows for expressing and enforcing syntactic constraints on the GP solutions. We applied CFG-based GP to enforce the dimensional consistency of empirical laws. Indeed, in virtually all physical applications, the domain variables are labelled with their dimensions (units of measurement), and the solution law must be consistent with respect to them (seconds and meters should not be added). Dimensional consistency allows for massive contractions of the GP search space; it significantly increases the accuracy and intelligibility of the empirical laws found.

A second limitation of GP is that it requires huge amounts of computational resources, even when the search space is properly constrained. This is blamed on the bloat phenomenon, resulting from the growth of non-coding branches (*introns*) in the GP individuals [1,10]. The bloat phenomenon adversely affects GP in two ways; on one hand, it might causes the early termination of the GP runs

due to the exhaustion of available memory; on the other hand, it significantly increases the fitness computation cost.

In this paper a new GP scheme addressing the bloat phenomenon is presented, which combines CFG-based GP and distribution-based evolution. In distribution-based evolution, an example of which is PBIL [11], the genetic pool is coded as a distribution on the search space; in each generation, the population is generated from the current distribution; and the distribution is updated from the best (and possibly the worst) individuals in the current population.

In this new scheme, termed SG-GP (for *Stochastic Grammar-based GP*), the distribution on the GP search space is represented as a stochastic grammar. It is shown experimentally that this scheme prevents the uncontrolled growth of introns. This result offers new hints into the bloat phenomenon.

The paper is organized as follows. The next section briefly summarizes context-free grammars (CFGs) and CFG-based GP, in order for the paper to be self contained. The principles of Distribution-based evolution are presented in section 3, and related works are discussed [12]. Stochastic Grammar based GP is detailed in Section 4. An experimental validation of SG-GP on real-world problems is reported in Section 5, and the paper ends with some perspectives for further research.

2 CFG-based GP

2.1 Context Free Grammars

A context free grammar describes the admissible constructs of a language by a 4-tuple $\{S, N, T, P\}$, where S is the start symbol, N the set of non-terminal symbols, T the set of terminal symbols, and P the production rules. Any expression is iteratively built up from the start symbol by rewriting non-terminal symbols into one of their derivations, as given by the production rules, until the expression contains terminals only. Fig. 1 shows the CFG describing the polynoms of variable X , to be compared with the standard GP description from the node set $\mathcal{N} = \{+, \times\}$ and terminal set $\mathcal{T} = \{X, \mathcal{R}\}$:

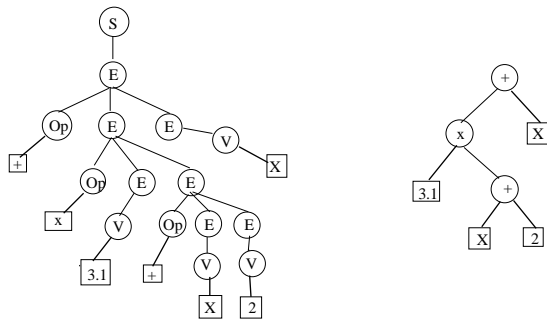
$$\begin{aligned}
 N &= \{ \langle exp \rangle, \langle op \rangle, \langle var \rangle \} \\
 T &= \{ +, \times, X, \mathcal{R} \} \quad // \mathcal{R} \text{ stands for any real-valued constant} \\
 P &= \left\{ \begin{array}{l} S := \langle exp \rangle ; \\ \langle exp \rangle := \langle op \rangle \langle exp \rangle \langle exp \rangle \mid \langle var \rangle ; \\ \langle op \rangle := + \mid \times ; \\ \langle var \rangle := X \mid \mathcal{R} ; \end{array} \right\}
 \end{aligned}$$

Fig.1. Context Free Grammar for polynoms of any degree of variable X

Note that *non-terminals* and *terminals* have different meanings in GP and in CFGs. GP terminals (resp. non-terminals) stand for domain variables and constants (resp. operators). CFGs terminals comprise domain variables, constants, and operators.

2.2 CFG-based GP

On one hand, CFGs allow one to express problem-specific constraints on the GP search space. On the other hand, the recursive application of derivation rules allows the build up of a *derivation tree* (Fig. 2), which can be thought of as an alternative representation for the expression tree. In this case, S stands for the start symbol, E for an expression, v for a variable and Op for an operator.



Derivation tree Parse tree
 Fig.2. Derivation tree and Corresponding Parse tree

Derivation trees can be manipulated using evolution operators. In order to ensure that CFG-compliant offspring are produced from CFG-compliant parents, crossover is restricted to swapping subtrees built on the same non-terminal symbol; mutation replaces a subtree by a new tree built on the same symbol [8,9]. These restrictions are quite similar to that of Strongly Typed GP [13].

2.3 Dimensionally-aware GP

As mentioned in the introduction, the discovery of empirical laws is easier when units of measurement are taken into account. These units can be expressed with respect to a set of elementary units, and represented as vectors (e.g. $Newton = mass \times length \times time^{-2}$ is represented as vector $[1, 1, -2]$). Restricting ourselves to a finite number of compound units, a non-terminal symbol is associated to any allowed compound unit. The associated derivation rule describes all possible ways for generating an expression of the given unit. An automatic grammar generator takes as input the elementary units and the set of compound units allowed, and produces the CFG describing all dimensionally consistent expressions in the search space¹. Although the CFG size is exponential, enforcing these restrictions linearly increases the crossover complexity in the worst case, and does not modify the mutation complexity.

Compared to most CFGs used in the GP literature [8], the dimensional-CFG is huge (several hundreds non-terminal symbols, several thousands of derivations). The inefficiency of CFG-GP in this frame, already reported by [14], was

¹ The production rule associated to the start symbol specifies the unit of the sought solution; it can also enforce the shape of the solution, according to the expert guess.

blamed on the initialization operator. This drawback was addressed by a specific, constrained grammar-based initialization process, building a CFG-compliant *and sufficiently diverse* initial population. The core of the procedure is a two-step process: a) for any given non-terminal symbol, all derivations compatible with the maximum tree-depth prescribed (ensuring that the final expression will have admissible size) are determined; b) the non-terminal symbol at hand is rewritten by uniformly selecting one compatible derivation (see [7] for more details).

3 Distribution-based Evolution

Contrasting with genetic evolution, distribution-based evolution deals with a high-level (intentional) description of the best individuals encountered so far, as opposed to the (extensional) description given by the current population itself. This intentional description is a probability distribution on the solution space, which is updated according to a set of rules.

As far as we know, the first algorithm resorting to distribution-based evolution is *Population-based Incremental Learning (PBIL)* [11], concerned with optimization in $\{0, 1\}^n$. In this scheme, distribution \mathcal{M} is represented as an element of $[0, 1]^n$, initialized to $\mathcal{M}_0 = (.5, \dots, .5)$.

At generation t , \mathcal{M}_t is used to generate the population from scratch, where the probability for any individual X to have its i -th bit set to 1 is given as the i -th component of \mathcal{M}_t . The best individual X_{best} in the current population is used to update \mathcal{M}_t by relaxation², with

$$\mathcal{M}_{t+1} = (1 - \epsilon)\mathcal{M}_t + \epsilon X_{best}$$

\mathcal{M}_t is also randomly perturbed (mutated) to avoid premature convergence.

This scheme has been extended to accommodate different distribution models and non-binary search spaces (see [15,16] among others).

Distribution-based evolution has been extended to GP through the *Probabilistic Incremental Program Evolution (PIPE)* system [12]. The distribution on the GP search space is represented as a Probabilistic Prototype Tree (PPT); in each PPT node stand the probabilities for selecting any variable and operator in this node. After the current individuals have been constructed and evaluated, the PPT is biased toward the current best and the best-so-far individuals. One feature of the PIPE system is that the PPT grows deeper and wider along evolution, depending on the size of the best trees, since the probabilities of each variable/operator have to be defined for each possible position in the tree.

4 Stochastic Grammars-based GP (SG-GP)

4.1 Overview

Distribution-based evolution actually involves three components: the representation (model) for the distribution; the exploitation of the distribution in order to

² Other variants use the best two individuals, and possibly the worst one too, to update the distribution.

generate the current population, which is analogous in spirit to the genetic initialization operator; the update mechanism, evolving the distribution according to the most remarkable individuals in the current population.

In CFG-GP, initialization proceeds by iteratively rewriting each non-terminal symbol; this is done by selecting a derivation in the production rule associated to the current non-terminal symbol (e.g. $\langle exp \rangle$ is either rewritten as a more complex expression, $\langle op \rangle \langle exp \rangle \langle exp \rangle$, or a leaf $\langle var \rangle$, Fig. 1). The selection is uniform (among the derivations compatible with the maximum tree size allowed, see Section 2.3). It comes naturally to encode the experience gained from the past generations, by setting selection probabilities on the derivations.

Representation. The distribution over the GP search space is represented as a stochastic grammar: each derivation d_i in a production rule is attached a weight w_i , and the chances for selecting derivation d_i are proportional to w_i .

Exploitation. The construction of the individuals from the current stochastic grammar is inspired from the CFG-GP initialization procedure. For each occurrence of a non-terminal symbol, all admissible derivations are determined from the maximum tree size allowed and the position of the current non-terminal symbol as in [7]; the selection of the derivation d_i is done with probability p_i , where

$$p_i = \begin{cases} \frac{w_i}{\sum_{k \in \text{admissible derivs.}} w_k} & \text{if } d_i \text{ is an admissible derivation} \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

This way, weights w_i need not be normalized.

Distribution update. After all individuals in the current population have been evaluated, the probability distribution is updated from the N_b best and N_w worst individuals according to the following rules: for each derivation d_i ,

- Let b denotes the number of individuals among the N_b best individuals that carry derivation d_i ; weight w_i is multiplied by $(1 + \epsilon)^b$;
- Let w denotes the number of individuals among the N_w worst individuals that carry derivation d_i ; weight w_i is divided by $(1 + \epsilon)^w$;
- Last, weight w_i is mutated with probability p_m ; the mutation either multiplies or divides w_i by factor $(1 + \epsilon_m)$.

All w_i are initialized to 1. Note that it does not make sense to have them normalized; they must be locally renormalized before use, depending on the current set of admissible derivations.

This distribution-based GP, termed SG-GP, involves five parameters besides the three standard GP parameters (Table 1).

4.2 Scalar and Vectorial SG-GP

In the above scheme, the genetic pool is represented by a vector \mathcal{W} , coding all derivation weights for all production rules. The storage of a variable length

Table 1. Parameters of Stochastic Grammar-based Genetic Programming

Parameter	Definition
Parameters specific to SG-GP	
N_b	Number of best individuals for probability update
N_w	Number of worst individuals for probability update
ϵ	Learning rate
p_m	Probability of mutation
ϵ_m	Amplitude of mutation
Canonical GP parameters	
P	Population size
G	Maximum number of generations
D_{max}	Maximum derivation depth

population is replaced by the storage of a single fixed size vector; this is in sharp contrast with canonical GP, and more generally, with all evolutionary schemes dealing with variable size individuals.

One limitation of this representation is that it induces a total order on the derivations in a given production rule. However, it might happen that derivation d_i is more appropriate than d_j in higher levels of the GP trees, whereas d_j is more appropriate in the bottom of the trees.

To take into account this effect, a distribution vector \mathcal{W}_i is attached to the i -th level of the GP trees (i ranging from 1 to D_{max}). This scheme is referred to as *Vectorial SG-GP*, as opposed to the previous scheme of *Scalar SG-GP*.

The distribution update in Vectorial SG-GP is modified in a straightforward manner; the update of distribution \mathcal{W}_i is only based on the derivations actually occurring at the i -th level among the best and worst individuals in the current population.

4.3 Investigations on intron growth

It have often been observed experimentally that the proportion of introns in the GP material grows exponentially along evolution [17]. As already mentioned, the intron growth is undesirable as it drains out the memory resources, and increases the total fitness computation cost.

However, it was also observed that pruning the introns in each generation significantly decreases the overall GP performances [1]. Supposedly, introns protect good building blocks from the destructive effects of crossover; as the useful part of the genome is condensed into a small part of the individual, the probability for a crossover to break down useful sections is reduced by the apparition of introns.

Intron growth might also be explained from the structure of the search space [10]. Consider all genotypes (GP trees) coding a given phenotype (program). There exists a lower bound on the genotype size (the size of the shortest tree coding the program); but there exists no upper bound on the genotype size (a long genotype can always be made longer by the addition of introns). Since

there are many more long genotypes than short ones, longer genotypes will be selected more often than shorter genotypes (everything else being equal, i.e. assuming that the genotypes are equally fit)³.

Last, intron growth might also be a mechanical effect of evolution. GP crossover facilitates the production of larger and larger trees: on one hand, the offspring average size is equal to the parent average size; on the other hand, short size offspring usually are poorly fit; these remarks together explain why the individual size increases along evolution.

Since the information transmission in SG-GP radically differs from that in GP, as there exists no crossover in SG-GP, there should be no occasion for building longer individuals, and no necessity for protecting the individuals against destructive crossover.

Experiments with SG-GP are intended to assess the utility of introns. If the intron growth is beneficial *per se*, then either SG-GP will show able to produce introns — or the overall evolution results will be significantly degraded. If none of these eventualities is observed, this will suggest that the role of introns has been overestimated.

5 Experimental validation

5.1 Test problem

The application domain selected for this study is related to the identification of rheological models. These problems have important applications in the development of new materials, especially for polymers and composite materials [19]. The target empirical law corresponds to the Kelvin-Voigt model, which consists of a spring and a dashpot in parallel (Fig. 3). When a constant force is applied, the response (displacement-time relation) is

$$u(t) = \frac{F}{K} \left(1 - e^{-\frac{Kt}{C}} \right)$$

Fitness cases (examples) are generated using random values of the material parameters K and C and loading F . The physical units for the domain variables and for the solution are expressed with respect to the elementary *mass*, *time* and *length* units (Table 2). Compound units are restricted as the exponent for each elementary unit ranges in $\{-2, -1, 0, 1, 2\}$. The dimensional grammar is generated as described in Section 2.3, with 125 non-terminal symbols and four operators (addition, multiplication, protected division and exponentiation). The grammar size is about 515 k.

³ To prevent or reduce this intron growth, a parsimony pressure might be added to the fitness function [18]; but the relative importance of the actual fitness and that of the parsimony term must be adjusted carefully. And the optimal trade-off might not be the same for the beginning and the end of evolution.

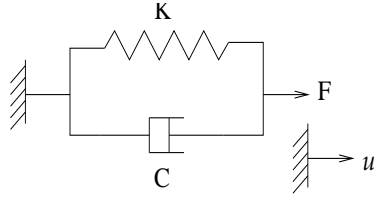


Fig. 3 Kelvin-Voigt Model

Physical units			
Quantity	mass	length	time
<i>Variables</i>			
F (Force)	+1	+1	-2
K (Elastic elements)	+1	0	-2
C (Viscous elements)	+1	0	-1
t (time)	0	0	+1
<i>Solution</i>			
u (displacement)	0	+1	0

Table 2. Physical Units

5.2 Experimental setting

SG-GP is compared⁴ with standard elitist GP. The efficiency of SG-GP is assessed with respect to the quality of solutions, and in terms of memory use. All results are averaged on 20 independent runs.

GP and SG-GP parameters are set according to a few preliminary experiments (Table 3). Canonical GP is known to work better with large populations and small number of generations [1]. Quite the contrary, SG-GP works better with a small population size and many generations. In both cases, evolution is stopped after 2,000,000 fitness evaluations.

SG-GP		GP	
Parameter	Value	Parameter	Value
Population size	500	Population size	2000
Max. number of generations	4000	Max. number of generations	1000
N_b	2	P(crossover)	0.9
N_w	2	P(mutation)	0.5
ϵ	0.001	Tournament size	3
P_m	0.001		
ϵ_m	0.01		

Table 3. Optimization parameters

5.3 Experimental results and parametric study

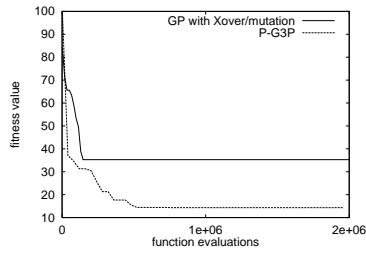


Fig. 4. Comparing GP and SG-GP

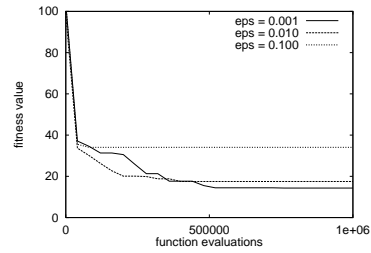


Fig. 5. Influence of the learning rate

⁴ Due to space limitations, the reader interested in the comparison of CFG-GP with GP is referred to [7].

Fig. 4 shows the comparative behaviors of canonical GP and SG-GP on the test identification problem. The influence of the learning rate ϵ is depicted on Fig. 5, and of the mutation amplitude ϵ_m on Fig. 6.a. Overall, better results are obtained with a low learning rate and a sufficiently large mutation amplitude; this can be interpreted as a pressure toward the preservation of diversity.

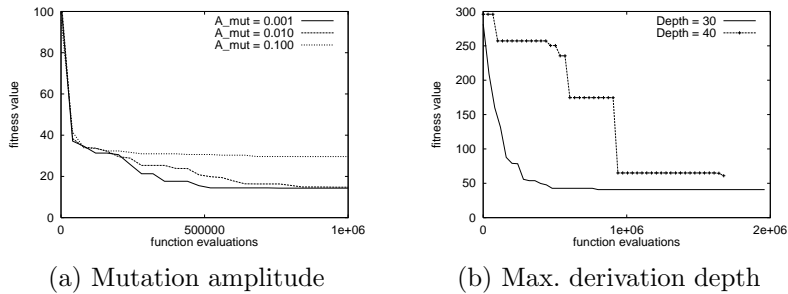


Fig. 6. Parametric study of SG-GP

The maximum derivation depth allowed D_{max} is also a critical parameter. Too short, and the solution will be missed, too large, the search will take a prohibitively long time. Fig. 6.b shows the solutions obtained with maximum derivation depths of 30 and 40. As could have been expected, the solution is found faster for $D_{max} = 30$.

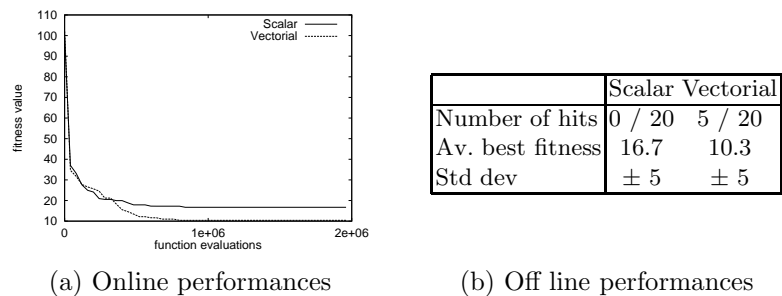


Fig. 7. Scalar vs Vectorial SG-GP

The advantage of using a vectorial distribution model against a scalar one, is illustrated on Fig. 7.a, as Vectorial SG-GP significantly improves on Scalar SG-GP. Table 7.b points out that vectorial SG-GP finds the target law (up to algebraic simplifications) after 2,000,000 fitness evaluations on 5 out of 20 runs, while no perfect match could be obtained with scalar SG-GP.

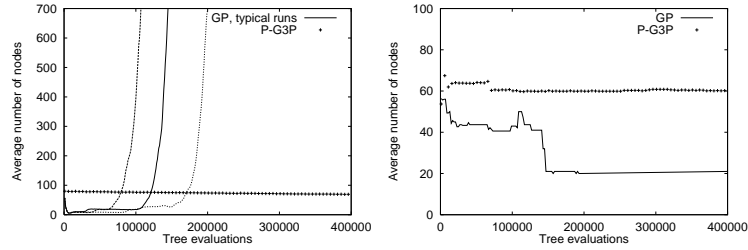
CFG-GP results, not shown here for space limitations, show that even scalar SG-GP is more efficient than CFG-GP (see [7] for more details).

5.4 Resisting the bloat

The most important experimental result is that SG-GP *does resist* the bloat, as it maintains an almost constant number of nodes. The average results over all individuals and 20 runs is depicted on Fig. 9.a.

In comparison is shown the number of nodes in GP (averaged on all individuals, but plotted for three typical runs for the sake of clarity). The individual size first drops in the first few generations; and after a while, it suddenly rises exponentially until the end of the run. The drop is due to the fact that many trees created by crossover in the first generations are either trivial solutions (very simple trees) or infeasible solutions which are rejected. The rise occurs as soon as large feasible trees emerge in the population.

As noted by [2], the size of the best individual is not correlated with the average size. Figure 8.b shows the average size of the best-so-far individual. Interestingly, SG-GP maintains an almost constant size for the best individual, which is slightly less than the average size. On the opposite, GP converges to a very small solution, despite the fact that most solutions are very large.



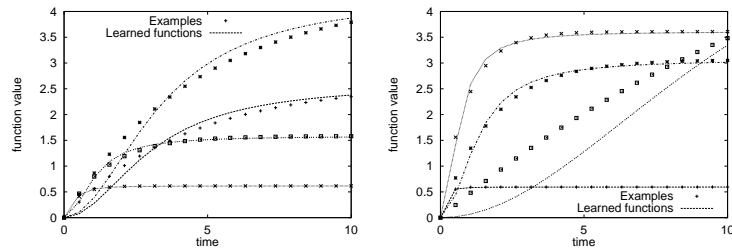
(a) Average individual size (b) Best individual size
 Fig. 8. Solution size with GP and SG-GP, averaged on 20 runs

5.5 Identification and Generalization

As mentioned earlier on, SG-GP found the target law in 5 out of 20 runs (up to algebraic simplifications). In most other runs, SG-GP converges toward a local optimum, a simplified expression of which is:

$$x(t) = \frac{2 * t^2 * \frac{F}{K}}{\frac{C}{K} * \frac{C}{K} + 2 * t^2} \quad (2)$$

This law is not on the path to the global optimum since the exponential is missing. However, the law closely fits the training examples, at least from an engineering point of view (Fig. 9.a).



(a) On training examples (b) On test examples
 Fig. 9. Correct Identification and Generalization with SG-GP

Even more important is the fact that SG-GP finds solutions which behaves well on test examples, i.e. examples generated after the target law, which have not been considered during evolution.

By construction, the target law perfectly fits the test examples. But the non-optimal law (Eq 2) also fits the test examples; the fit is quite perfect in three out of four cases, and quite acceptable, from an engineer's point of view, in the last case.

6 Conclusion

In this paper was presented a novel Genetic Programming scheme, combining grammar-based GP [8,9,7] and distribution-based evolution [11], termed SG-GP for Stochastic Grammar-based Genetic Programming. SG-GP differs from the PIPE system [12] as the distribution model used is based on stochastic grammars, which allows for overcoming one main limitation of GP, i.e. the bloat phenomenon.

Intron growth was suggested to be unavoidable for program induction methods with fitness-based selection [10].

This conjecture is infirmed by SG-GP results on a real-world like problem. Indeed, more intensive experiments are needed to see the limitations of the SG-GP scheme.

Still, SG-GP successfully resisted the intron growth on the problem considered, in the following sense.

First of all, SG-GP shows good identification abilities, as the target law was discovered in 5 out of 20 runs, while it was never discovered by canonical GP.

Second, SG-GP shows good generalization abilities; even in the cases where the target law was missed, the solutions found by SG-GP have good predictive accuracy on further examples (not considered during the learning task).

Last, these identification and generalization tasks are successfully completed by exploring individuals with constant size. No intron growth was observed; the overall memory requirements were lower by several orders of magnitude, than for canonical GP.

These results suggest that intron growth is not necessary to achieve efficient non parametric learning in a fitness-based context, but might rather be a side effect of crossover-based evolution.

Further research is concerned with examining the actual limitations of SG-GP through more intensive experimental validation. Efforts will be devoted to the parametric optimization problem (find the constants) coupled with non-parametric optimization.

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